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14. ABSTRACT

Summary: With respect to our modeling of condensation in supersonic expansions, we have used molecular dynamics to derive condensation based models for DSMC for non-Lennard Jonesian gases such as water, carbon dioxide, and ammonia, common combustion products found in rocket plumes. The challenge was to incorporate charge polarization terms in the cluster potential, develop and automate a strategy for recognizing the formation of clusters in an MD study of a supersonic expansion, and utilize a parallel MD code to deduce the important cluster formation mechanism in a large scale MD simulation of a jet expansion. In addition, we have extended our research to model heterogeneous condensation, a necessary feature for realistic plume flows which often include multiple species types. The developed MD models have been incorporated into the DSMC simulations, a process that takes the fine-grained simulation results and transfers them to the propulsion/nozzle system level. DSMC simulations have been compared with published Raman and Rayleigh scattering laboratory measurements, high lighting the need for this data for more molecular systems

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PENNSTATE

Department of Aerospace Engineering

Inter-office Memorandum

TO	Dr. Mitat A. Birkan
FROM	Deborah Levin, Prof. of Aerospace Engineering
SUBJECT	Final Report for Development of Improved Molecular Excitation Models - FA9550-06-1-0150
DATE	5 February 2010

This report presents the major technical accomplishments of the AFOSR grant entitled: "Development of Improved Molecular Excitation Models for the Modeling of High Altitude Space Plume Radiation" for calendar year 2009.

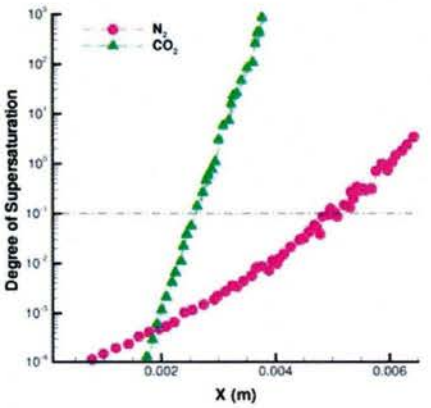
The report is subdivided into two sections that discuss the highlights of some of the research that has been performed this year. Please let me know if you would like more detail or information.

(1) Progress on modeling homogeneous and heterogeneous condensation of non- Lennard-Jonesian Gases

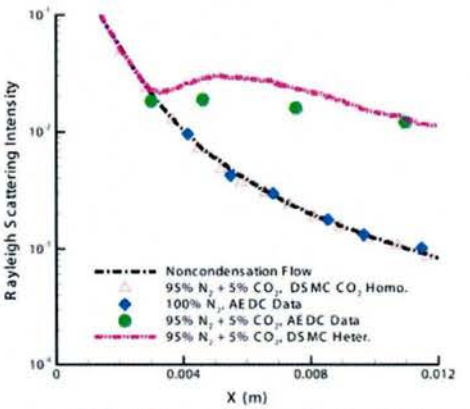
Summary: With respect to our modeling of condensation in supersonic expansions, we have used molecular dynamics to derive condensation based models for DSMC for non-Lennard Jonesian gases such as water, carbon dioxide, and ammonia, common combustion products found in rocket plumes. The challenge was to incorporate charge polarization terms in the cluster potential, develop and automate a strategy for recognizing the formation of clusters in an MD study of a supersonic expansion, and utilize a parallel MD code to deduce the important cluster formation mechanism in a large scale MD simulation of a jet expansion. In addition, we have extended our research to model heterogeneous condensation, a necessary feature for realistic plume flows which often include multiple species types. The developed MD models have been incorporated into the DSMC simulations, a process that takes the fine-grained simulation results and transfers them to the propulsion/nozzle system level. DSMC simulations have been

compared with published Raman and Rayleigh scattering laboratory measurements, high lighting the need for this data for more molecular systems.

A Research Highlight: The figure shows the super-saturation properties of a carbon dioxide – nitrogen gas plume mixture (a) and a comparison of DSMC simulations of the heterogeneous condensation flow with data taken from AEDC (b). The degree of super saturation is the ratio of the condensable gas saturation pressure to the gas pressure. As the plume expands the degree of saturation for all condensable gases will exponentially increase because the gas pressure decreases as the super saturation pressure increases because the gas temperature is decreasing. For a gas mixture of carbon dioxide and nitrogen, the carbon dioxide will condense earlier in the plume expansion, as is shown in the figure. Therefore even a small amount of (5%) carbon dioxide clusters serve as seed nuclei for subsequent condensation of molecular nitrogen clusters. Rayleigh scattering intensity data of a carbon dioxide/nitrogen mixture shows that cluster formation cannot be observed in a pure nitrogen plume expansion, however, just a small amount of carbon dioxide is sufficient to cause heterogeneous condensation (purple curve in (b)). Molecular dynamics was used to determine the nucleation mechanism and rate. Initially two carbon dioxide molecules collide and form a metastable dimer. The meta-stable dimer was found to have a sufficiently long life time that either another carbon dioxide molecule, but, more likely, a nitrogen molecule collides to form a stable trimer. Subsequent collisions of the trimer with either type of molecule can lead to the creation of larger clusters by sticking. The green symbol are the DSMC predicted Rayleigh scattering intensities, using the MD derived condensation rates and sticking probabilities. The agreement between the measurements and simulation are good.



(a) Species N_2 and CO_2 degree of supersaturation along the plume centerline



(b) Rayleigh scattering intensity along the plume centerline (DSMC simulation results and AEDC experimental data)

Publications:

The archival papers in support of this research:

J. Zhong, N. Moghe, Z. Li, and D. Levin, "A Unimolecular Evaporation Model for Simulating Argon Condensation Flows in DSMC," *Physics of Fluids*, Vol. 21, p. 036101, 2009.

Z. Li, J. Zhong, D. Levin and B. Garrison, "Development of Homogeneous Water Condensation Models Using Molecular Dynamics," *AIAA Journal*, May Vol. 47, Number 5, pp. 1241-1251, 2009.

Z. Li, J. Zhong, D. Levin, and B. Garrison, "Kinetic Nucleation Model for Free-Expanding Water Condensation Plume Simulations," *Journal of Chemical Physics*, 7 May 7, 2009, Vol. 130, Issue, 17, URL:http://link.aip.org/link/?JCP/130/174309 DOI: 10.1063/1.3129804.

Li, Z., Zhong, J., and Levin, D. "Modeling of CO_2 Homogeneous and heterogeneous Condensation Plumes," *The Journal of Physical Chemistry*, special edition, Publication Date (Web): October 16, 2009, DOI: 10.1021/jp9040698.

In addition, the following conference papers were written and presented and some of them will become archival papers in the following calendar year:

Z. Li and D. Levin, "Development of Ammonia Cluster-Cluster Coalescence Model Using Molecular Dynamics," AIAA Paper No. 2009-3748, 41st AIAA Thermophysics Conference, 22-25 June 2009, San Antonio, Texas, manuscript in preparation.

D. Levin and Z. Li, "Challenges of Modeling Multi-scale Condensation Flows Using Kinetic Simulation Approaches," invited talk at DSMC2009 Workshop, Santa Fe, New Mexico, September 14, 2009.

Z. Li, B. Garrison, and D. Levin, AIAA 2008-4420 entitled "Kinetic Nucleation Model for Free-Expanding Water Condensation Plume Simulations," won the 2009 AIAA David Weaver Best Student Paper award.

(2) Progress on the development of a Collision-limiter DSMC scheme for modeling micronozzle propopulsion:

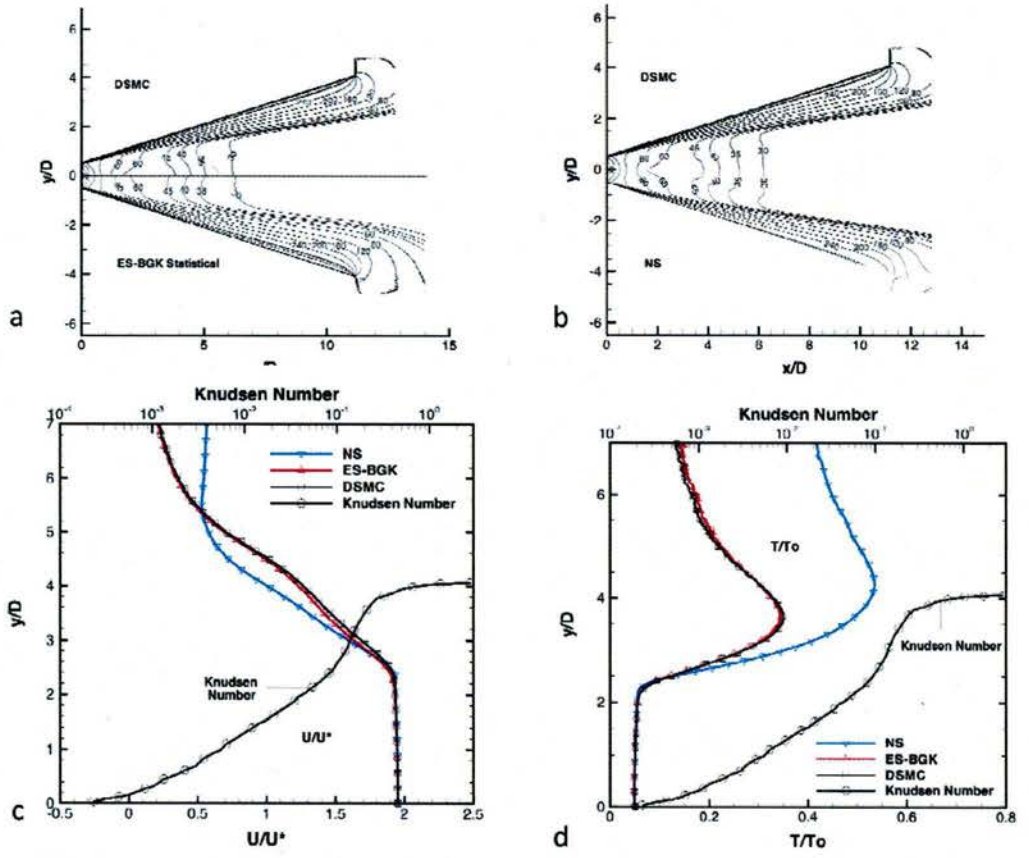
Summary: Our present method of implementing condensation in a supersonic expansion to vacuum is to assume that condensation occurs downstream of the nozzle or orifice exit, *i.e.*, in a region where the flow is supersonic. Previously we have used CFD to model the dense flow from the exit to a region where the Knudsen number is sufficiently large that the DSMC calculation may be started. This transference of information from the continuum/NS calculations to the DSMC is straightforward and is accomplished by using a starting surface. However, there are many examples for plenum conditions higher than 1 atm where condensation occurs upstream of the usual DSMC starting surface, occurs inside the nozzle, or has a sufficiently complex geometry that the construction of a starting surface is non-trivial. In previous progress reports we presented a collision-limiter method known as eDSMC. Comparison of eDSMC with DSMC simulations of nozzle flowfields (both without condensation) showed that eDSMC was able to reproduce the inviscid core region, but, was poor in the viscous shocklayer. eDSMC, restricted to the inviscid core, combined with DSMC was found to provide a factor of ten speed up over pure DSMC, but it was deemed insufficiently inaccurate to use for condensing flows. For this reason the Bhatngar-Gross-Krook (BGK) model for kinetic flows has been implemented. For viscous flows at high enough density the Boltzmann equation collision term can be simplified by assuming that it has the form of relaxation to an equilibrium distribution. The computational approach is more efficient than DSMC because the particle collisions are not performed over and over again. Specifically we use, the Ellipsoidal (ES)-BGK method, an extension of the BGK method, formulated to correct the unphysical value of the unity Prandtl number in the BGK method. The research highlight discusses the nozzle modeling without condensation. However, AIAA-2010-0818 paper given a few weeks ago demonstrates the use of BGK in modeling a carbon dioxide condensating flow at high pressures. The results presented were preliminary and final reports will be reported next year.

A Research Highlight: The figures below correspond to a flow through a conical nozzle with a Re=12300, a case usually not attempted by DSMC due to its intensive computational nature. However, because we will show that the NS, normally considered the correct approach, also has problems in the nozzle back flow region, extremely expensive DSMC calculations were undertaken for the basis of comparison and are considered "truth".

The set of four figures below illustrate the high lights of the research. Plots (a) and (b) show a comparison of the statistical ES-BGK vs. DSMC and NS vs. DSMC gas

temperature contours. The flow exhibits the typical features of a supersonic nozzle expansion, i.e., an inviscid core and a thick boundary layer. Also, since the present case is for a pressure 10 times higher usually modeled with DSMC, there is good agreement between the solutions of the NS and DSMC methods. However even at this high pressure, the agreement slightly worsens in the relatively rarefied portions of the flow, near the nozzle exit and close to the boundary layer. However, because the NS and DSMC solutions are so close, there will be no significant difference in the thrust predicted by either method, thereby, reducing the rationale for developing a more efficient statistical particle method at high pressures. In other words, although the ES-BGK method will have better efficiency compared to DSMC, the former will not be as computationally efficient as NS.

However, if degree of spacecraft contamination due to plume backflow is the aim of the calculation, the NS method cannot be used. Plots (c) and (d) show the variation of the x component of velocity and temperature across a plane normal to the nozzle centerline at x/D = 0.85 downstream of the nozzle exit plane. Also, the variation of local Knudsen number based on the density gradient, is shown in the figure and it can be seen that the variation is large in the nozzle lip region, even for this high pressure case. The NS solutions are seen to deviate from that of DSMC. The figure shows that although there are regions with Knudsen number well within the continuum, deviation between the two solutions is significant, particularly, in the region where $Kn < 0.1$. The disagreement between the NS and DSMC is as much as 20% in both velocity and temperature, whereas the statistical ES-BGK method shows only a discrepancy of less than 4% from the DSMC, which is within the numerical accuracy. The back flow rate, calculated at the nozzle exit plane, predicted by the NS solution is zero, whereas both DSMC and ES-BGK methods predict a value of 18×10^{-9} kg/s (compared to the total mass flow rate of 202.2×10^{-6} kg/s through the nozzle).



Publications:

The archival papers in support of this research:

R. Kumar, E. Titov, D. Levin, N. Gimelshein, and S. Gimelshein, "Assessment of BGK Approaches to Modeling of Nozzle Flows in the Near Continuum Regime," accepted to AIAA Journal, January 26, 2010.

R. Kumar, E. Titov, and D. Levin, "Study of Compressible Laminar Boundary Layer Flows with Statistical BGK Approaches," accepted for publication in the Journal of Thermophysics and Heat Transfer, Nov. 2009.

R. Kumar, E. Titov, and D. Levin, "Reconsideration of Planar Couette Flows Using a Statistical Approach to the BGK Model Kinetic Equation," accepted for publication in the Journal of Thermophysics and Heat Transfer, Dec. 2009.

In addition, the following conference papers were written and presented and some of them will become archival papers in the following calendar year:

R. Kumar, E. Titov, and D. Levin, "Comparison of Statistical BGK and DSMC Methods with Theoretical Solutions for Two Classical Fluid Flow Problems," AIAA Paper No. 2009-3740, 41st AIAA Thermophysics Conference, 22-25 June 2009, San Antonio, Texas.

R. Kumar, Z. Li and D. Levin, "Modeling of CO_2 Condensation in the High Pressure Flows Using the Statistical BGK Method," AIAA-2010-0818, 48th AIAA Aerospace Sciences Meeting, 4-7 January 2010, Orlando, Florida.

Z. Li, A. Borner, and D. Levin, R. Jansen, S. Gimelshein, M. Zeifman, and I. Wysong, "Sensitivity and Accuracy Analysis for Kinetic Modeling of Homogeneous Condensation in Plumes," AIAA-2010-0985, 48th AIAA Aerospace Sciences Meeting, 4-7 January 2010, Orlando, Florida.